# Optimization of nonlocal time-delayed feedback controllers

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Abstract A class of Pyragas type nonlocal feedback controllers with time-delay is investigated for the Schlögl model. The main goal is to find an optimal kernel in the controller such that the associated solution of the controlled equation is as close as possible to a desired spatio-temporal pattern. An optimal kernel is the solution to a nonlinear optimal control problem with the kernel taken as control function. The well-posedness of the optimal control problem and necessary optimality conditions are discussed for different types of kernels. Special emphasis is laid on time-periodic functions as desired patterns. Here, the cross correlation between the state and the desired pattern is invoked to set up an associated objective functional that is to be minimized. Numerical examples are presented for the 1D Schlögl model and a class of simple step functions for the kernel.

**Keywords** Schlögl model, Nagumo equation, Pyragas type feedback control, nonlocal delay, controller optimization, numerical method

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#### 1 Introduction

In this paper, we consider a class of nonlocal feedback controllers with application to the control of certain nonlinear partial differential equations. The research on feedback control laws of this type has become quite active in theoretical physics for stabilizing periodic wave-type solutions of reaction-diffusion systems such as the Schlögl model (also known as Nagumo or Chafee-Infante equation) or the FitzHugh-Nagumo system.

The controllers can be characterized as follows: First of all, they are generalizations of Pyragas type controllers that became very popular in the past. We refer to [21], [22], and the survey volume [25]. In [21], a time-delayed feedback was suggested as a method to stabilize unstable periodic orbits embedded in a chaotic attractor in the context of ordinary differential equations (chaos control). In the simplest form of Pyragas type feedback control, applied to partial differential equations, the difference of the current state u(x,t) and the retarded state  $u(x,t-\tau)$ , multiplied with a real number  $\kappa$ , is taken as control, i.e. the feedback control f is

$$f(x,t) := \kappa \left( u(x,t) - u(x,t-\tau) \right),$$

where  $\tau$  is a fixed time delay and  $\kappa$  is the feedback gain. A feedback of Pyragas type can be applied to stabilize periodic orbits of dynamical systems. If, for instance, a solution u has the time period  $\tau$ , then f vanishes so that the feedback is called *noninvasive*. In contrast to well known Riccati or Lyapunov type stabilization techniques, Pyragas type feedback control does not require the knowledge of a reference solution that is to be stabilized. It is sufficient to know the existence of a periodic solution with period  $\tau$ . This method has been applied to a great variety of systems, e.g., lasers, optoelectronic oscillators, chemical reactions, cardiac dynamics etc., cf. [12].

In the nonlocal generalization we consider in this paper, the feedback control is set up by an integral operator of the form

$$f(x,t) := \kappa \left( \int_0^T g(\tau)u(x,t-\tau) d\tau - u(x,t) \right). \tag{1}$$

Here, varying time delays appear in a distributed way. Depending on the particular choice of the kernel g, various spatio-temporal patterns of the controlled solution u can be achieved. In particular, stable periodic patterns can be generated. We refer to [2,20,27], and [26] with application to the Schlögl model and to [1,17,30] with respect to control of ordinary differential equations.

Our main goal is the selection of the kernel g in an optimal way. We want to achieve a desired spatio-temporal pattern for the resulting state function and look for an optimal feedback kernel g to approximate this pattern as closely as possible. For this purpose, in the second half of the paper we will concentrate on a particular choice of g as a step function.

We are optimizing feedback controllers but we shall apply methods of optimal control to achieve our goal. This leads to new optimal control problems for reaction-diffusion equations containing nonlocal terms with time delay in the state equation. We develop the associated necessary optimality conditions and discuss numerical approaches for solving the problems posed. Working on this class of problems, we observed that standard quadratic tracking type objective functionals are possibly not the right tool for approximating desired time-periodic patterns. We found out that the so-called cross correlation partially better fits to our goals. We report on our numerical tests at the end of this paper.

This research contributes results to the optimal control of nonlinear reaction diffusion equations, where wave type solutions such as traveling wave fronts or spiral waves occur in unbounded domains. We mention the papers [3, 4,9] on the optimal control of systems that develop spiral waves or [14–16] on systems with heart medicine as background. Moreover, we refer to [5,7], where different numerical and theoretical aspects of optimal control of the Schlögl or FitzHugh-Nagumo equations are discussed. It is a characteristic feature of such systems that the computed optimal solutions might be unstable with respect to perturbations in the data, in particular initial data.

Feedback control aims at generating stable solutions. Various techniques of feedback control are known, we refer only to the monographies [10,18,19, 28] and to the references cited therein. Moreover, we mention [13] on feedback stabilization for the Schlögl model. Pyragas type feedback control is one associated field of research that became very active, cf. [25] for an account on current research in this field. In associated publications, the feedback control laws were considered as given. For instance, the kernel in nonlocal delayed feedback was given and it was studied what kind of patterns arise from different choices of the kernel.

The novelty of our paper is that we study an associated inverse (say design) problem: Find a kernel such that the associated feedback solution best approximates a desired pattern. We do not investigate the question, whether and under which conditions the state function u approaches a periodic solution as  $t \to \infty$ .

#### 2 Two models of feedback control

We consider the following semilinear parabolic equation with reaction term R and control function (forcing) f,

$$\partial_t u - \Delta u + R(u) = f \tag{2}$$

subject to appropriate initial and boundary conditions in a spatio-temporal domain  $Q := \Omega \times (0, T)$ . Using a feedback control in the form (1), we arrive at the following nonlinear initial-boundary value problem that includes a nonlocal

term with time delay,

$$\partial_t u(x,t) - \Delta u(x,t) + R(u(x,t)) = \kappa \left( \int_0^T g(\tau) u(x,t-\tau) d\tau - u(x,t) \right) \text{in } Q,$$

$$u(x,s) = u_0(x,s) \qquad \text{in } \Omega \times [-T,0],$$

$$\partial_n u(x,t) = 0 \qquad \text{on } \Sigma,$$
(3)

where,  $\partial_n$  denotes the outward normal derivative on  $\Gamma = \partial \Omega$  and we introduced  $\Sigma := \Gamma \times (0,T)$ . We want to determine a feedback kernel  $g \in L^{\infty}(0,T)$  such that the solution u to (3) is as close as possible to a desired function  $u_d$ . The function g will have to obey certain restrictions, namely

$$0 \le g(t) \le \beta$$
 a.e. on  $[0, T]$ , (4)

$$\int_0^T g(s) \, ds = 1,\tag{5}$$

where  $\beta > 0$  is a given (large) positive constant. This upper bound is chosen to have a uniform bound for g. It is needed for proving the solvability of the optimal control problem.

We shall present the main part of our theory for the general type of g defined above. In our numerical computations, however, we will concentrate on functions g of the following particular form: We select  $t_1$ ,  $t_2$  such that  $0 \le t_1 < t_2 \le T$ ,  $t_2 - t_1 \ge \delta > 0$  and define

$$g(t) = \begin{cases} \frac{1}{t_2 - t_1}, t_1 \le t \le t_2 \\ 0, & \text{elsewhere.} \end{cases}$$
 (6)

It is obvious that g satisfies the constraints (4),(5) with  $\beta = 1/\delta$ . Using this form for g, we end up with the particular feedback equation

$$\partial_t u(x,t) - \Delta u(x,t) + R(u(x,t)) = \kappa \left( \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} u(x,t-\tau) \, d\tau - u(x,t) \right). \tag{7}$$

In (7), we will also vary  $\kappa$  in the state equation as part of the control variables to be optimized. In contrast to this,  $\kappa$  is assumed to be fixed in the model with a general control function g. In the special model, we have a restricted flexibility in the optimization, because only the real numbers k,  $t_1$ ,  $t_2$  can be varied. Yet, we are able to generate a class of interesting time-periodic patterns.

Throughout the paper we will rely on the following

**Assumptions.** The set  $\Omega \subset \mathbb{R}^N$ ,  $N \leq 3$ , is a bounded Lipschitz domain; for N=1, we set  $\Omega=(a,b)$ . By T>0, a finite terminal time is fixed. In theoretical physics, also the choice  $T=\infty$  is of interest. However, we do not investigate the associated analysis, because an infinite time interval requires the use of more complicated function spaces. Moreover, the restriction to a bounded interval fits better to the numerical computations. Throughout the

paper, we use the notation  $Q:=\Omega\times(0,T)$  and  $\Sigma=\Gamma\times(0,T)$ . for the space-time cylinder.

Remark 1 We will often use the term "wave type solution" or "traveling wave". This is a function  $(x,t) \mapsto u(x,t)$  that can be represented in the form u(x,t) = v(x-ct) with some other smooth function v. Here, c is the velocity of the wave type solution. Such solutions are known to exist in  $\Omega = \mathbb{R}$  but not in in a bounded interval  $\Omega = (a,b)$ .

In our paper, the terms "wave type solution" or "traveling wave" stand for solutions of the Schlögl model in the bounded domain (a, b). We use these terms, since the computed solutions exhibit a similar behavior as associated solutions in  $\Omega = \mathbb{R}$ .

The reaction term R is defined by

$$R(u) = \rho (u - u_1)(u - u_2)(u - u_3), \tag{8}$$

where  $u_1 \leq u_2 \leq u_3$  and  $\rho > 0$  are fixed real numbers. In our computational examples, we will take  $\rho := 1$ . The numbers  $u_i$ ,  $i = 1, \ldots, 3$ , define the fixed points of the (uncontrolled) Schlögl model (2). In view of the time delay, we have to provide initial values  $u_0$  for u in the interval [-T, 0] for the general model (3) and in  $[-t_2, 0]$  for the special model (7). We assume  $u_0 \in C(\bar{\Omega} \times [-T, 0])$  or  $u_0 \in C(\bar{\Omega} \times [-t_2, 0])$ , respectively. The desired state  $u_d$  is assumed to be bounded and measurable on Q.

## 3 Well-posedness of the feedback equation

In this section, we prove the existence and uniqueness of a solution to the general feedback equation (3). To this aim, we first reduce the equation to an inhomogeneous initial-boundary value problem. For  $t \in [0, T]$ , we write

confidence as initial-boundary value problem. For 
$$t \in [0,T]$$
, we write 
$$\int_0^T g(\tau)u(x,t-\tau)\,d\tau = \int_0^t g(\tau)u(x,t-\tau)\,d\tau + \underbrace{\int_t^T g(\tau)u(x,t-\tau)\,d\tau}_{=:U_g(x,t)}$$
$$= \int_0^t g(\tau)u(x,t-\tau)\,d\tau + U_g(x,t).$$

The function  $U_g$  is associated with the fixed initial function  $u_0$  and is defined by

$$U_g(x,t) = \int_t^T g(\tau)u_0(x,t-\tau) d\tau;$$

notice that we have  $t-\tau \leq 0$  in the integral above. By the assumed continuity of  $u_0$ , the function  $U_g$  belongs to  $C(\bar{\varOmega} \times [0,T])$ . The mapping  $g \mapsto U_g$  is linear and continuous from  $L^{\infty}(0,T)$  to  $C(\bar{\varOmega} \times [0,T])$ , hence it is also Fréchet-differentiable. The derivative  $\partial_g U_g$  is given by

$$(\partial_g U_g h)(x,t) = \int_t^T h(\tau) u_0(x,t-\tau) d\tau.$$

Next, for given  $g \in L^2(0,T)$ , we introduce a linear integral operator  $K(g): L^2(Q) \to L^2(Q)$  by

$$(K(g)u)(x,t) := \int_0^t g(\tau)u(x,t-\tau) d\tau. \tag{9}$$

Substituting  $s = t - \tau$ , we obtain the equivalent representation

$$(K(g)u)(x,t) = \int_0^t g(t-s)u(x,s) ds.$$

Inserting  $U_g$  and K(g) in the state equation (3), we obtain the following non-local initial-boundary value problem:

$$\begin{cases}
\partial_t u - \Delta u + R(u) + \kappa u - \kappa K(g) u = \kappa U_g & \text{in } Q, \\
u(x,0) = u_0(x,0) & \text{in } \Omega, \\
\partial_n u = 0 & \text{on } \Sigma.
\end{cases}$$
(10)

In the next theorem, we use the Sobolev space

$$W(0,T) = L^2(0,T; H^1(\Omega)) \cap H^1(0,T; L^2(\Omega)).$$

**Theorem 1** For all  $g \in L^{\infty}(0,T)$ ,  $U_g \in L^p(Q)$ ,  $p > \frac{5}{2}$ , and  $u_0 \in C(\bar{\Omega} \times [-T,0])$ , the problem (10) has a unique solution  $u \in W(0,T) \cap C(\bar{Q})$ .

*Proof* We use the same technique that was applied in [8] to show the existence and continuity of the solution to the FitzHugh-Nagumo system. Let us mention the main steps. First, we apply a simple transformation that is well-known in the theory of evolution equations. We set

$$u = e^{\lambda t} v$$

with some  $\lambda > 0$ . This transforms the partial differential equation in (10) to an equation for the new unknown function v,

$$v_t - \Delta v + e^{-\lambda t} R(e^{\lambda t} v) + (\lambda + \kappa) v = \kappa K_{\lambda}(g) v + e^{-\lambda t} \kappa U_g, \tag{11}$$

where the integral operator  $K_{\lambda}(g)$  is defined by

$$(K_{\lambda}(g)v)(x,t) = \int_0^t e^{-\lambda(t-s)}g(t-s)v(x,s) ds.$$

If  $g \in L^{\infty}(0,T)$ , then both operators K(g) and  $K_{\lambda}(g)$  are continuous linear operators in  $L^{p}(Q)$ , for all  $p \geq 1$ . Moreover, due to the factor  $e^{-\lambda(t-s)}$ , the norm of  $K_{\lambda}(g): L^{2}(Q) \to L^{2}(Q)$  tends to zero as  $\lambda \to \infty$ . We obtain

$$||K_{\lambda}(g)||_{\mathcal{L}(L^{2}(Q))} \le \frac{c}{\sqrt{\lambda}} ||g||_{L^{\infty}(0,T)}$$
 (12)

with some constant c > 0. To have this estimate, we assumed in (4) that g is uniformly bounded by the constant  $\beta$ . If  $\lambda$  is sufficiently large, then we have

$$\int_Q \left[e^{-\lambda t} R(e^{\lambda t} v) + (\lambda + \kappa) v - \kappa K_\lambda(g) v\right] v \, dx dt \ge \frac{\lambda}{2} \|v\|_{L^2(Q)}^2 \quad \forall v \in L^2(Q),$$

because the coercive term  $(\lambda + \kappa)v$  in the left side is dominating the other terms, cf. [8].

With this inequality, an a priori estimate can be derived in  $L^2(Q)$  for any solution v of the equation (10). Now, we can proceed as in [8]: A fixed-point principle is applied in  $L^2(Q)$  to prove the existence and uniqueness of the solution v that in turn implies the same for u. For the details, the reader is referred to [8], proof of Theorem 2.1. However, we mention one important idea: Thanks to (12), the term  $(\lambda + \kappa)$  absorbes the non-monotone terms in the equation (11) so that, in estimations, equation (11) behaves like the parabolic equation

$$v_t - \Delta v + \tilde{R}(v) = F$$

with a monotone non-decreasing nonlinearity  $\tilde{R}$  and given right-hand side  $F \in L^p(Q)$ , p > 5/2. This fact can be exploited to verify, for each r > 0, the existence of a constant  $C_r > 0$  with the following property: If  $g \in L^{\infty}(Q)$  obeys  $\|g\|_{L^{\infty}(Q)} \leq r$  and u is the associated solution to (3), then

$$||u||_{L^{\infty}(Q)} \le C_r. \tag{13}$$

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#### 4 Analysis of optimization problems for feedback controllers

## 4.1 Definition of two optimization problems

General kernel as control

Let a desired function  $u_d \in L^{\infty}(Q)$  be given. In our later applications,  $u_d$  models a desired spatio-temporal pattern. Moreover, we fix a non-negative function  $c_Q \in L^{\infty}(Q)$ . This function is used for selecting a desired observation domain. We consider the feedback equation (3) and want to find a kernel g such that the associated solution u approximates  $u_d$  as close as possible in the domain of observation. This goal is expressed by the following functional  $j: L^2(Q) \times L^{\infty}(0,T) \to \mathbb{R}$  that is to be minimized,

$$j(u,g) := \frac{1}{2} \iint_{Q} c_{Q}(u - u_{d})^{2} dx dt + \frac{\nu}{2} \int_{0}^{T} g^{2}(t) dt.$$

Here,  $\nu \geq 0$  is a Tikhonov regularization parameter that is introduced for convenience. In our numerical tests, we observed that this regularization is not needed for the numerical stability. The standard choice of  $c_Q$  is  $c_Q(x,t)=1$  for all  $(x,t)\in Q$ . Another selection will be applied for periodic functions  $u_d$ :

c(x,t) = 1 for all  $(x,t) \in Q$  with  $t \ge T/2$  and c(x,t) = 0 for all  $(x,t) \in Q$  with t < T/2.

By Theorem 1, to each  $g \in L^{\infty}(0,T)$  there exists a unique associated state function u that will be denoted by  $u_g$ . Then j does only depend on g and we obtain the reduced objective functional J,

$$J: g \mapsto j(u_q, g).$$

Therefore, our general optimization problem can be formulated as follows:

$$\min_{g \in C} J(g) := \frac{1}{2} \iint_{Q} c_{Q} (u_{g} - u_{d})^{2} dx dt + \frac{\nu}{2} \int_{0}^{T} g^{2}(t) dt,$$
 (PG)

where  $C \subset L^{\infty}(0,T)$  is the convex and closed set defined by

$$C := \left\{ g \in L^{\infty}(0,T) : \ 0 \le g(t) \le \beta \ \text{ a.e. in } [0,T] \text{ and } \int_{0}^{T} g(t) \, dt = 1. \right\}$$

Notice that C is a weakly compact subset of  $L^2(0,T)$ . The restrictions on g are motivated by the background in mathematical physics. In particular, the restriction on the integral of g guarantees that

$$\int_0^T g(\tau)u(x,t-\tau)\,d\tau - u(x,t) = 0,$$

if  $u(x, t - \tau) = u(x, t)$  in Q. By the definition of  $u_g$ , the optimization is subject to the state equation (3).

Special kernel as control

The other optimization problem we are interested in, uses the particular form (6) of the kernel g,

$$\min_{0 \le t_1 < t_2 \le T} J_S(\kappa, t_1, t_2) := \frac{1}{2} \iint_Q c_Q (u_{(\kappa, t_1, t_2)} - u_d)^2 \, dx dt + \frac{\nu}{2} (t_1^2 + t_2^2 + \kappa^2),$$

where  $u_{(\kappa,t_1,t_2)}$  is the solution of (7) for a given triplet  $(\kappa,t_1,t_2)$ . This problem might fail to have an optimal solution, because the set of admissible triplets  $(\kappa,t_1,t_2)$  is not closed. Notice that we need  $t_1 < t_2$  in (7). Therefore, we fix  $\delta > 0$  and define the slightly changed admissible set

$$C_{\delta} := \{ (\kappa, t_1, t_2) \in \mathbb{R}^3 : 0 \le t_1 < t_2 \le T, t_2 - t_1 \ge \delta, \ \kappa \in \mathbb{R} \}$$

that is compact. In this way, we obtain the special finite-dimensional optimization problem for step functions g,

$$\min_{(\kappa, t_1, t_2) \in C_{\delta}} J_S(\kappa, t_1, t_2) := \frac{1}{2} \iint_Q c_Q (u_{(\kappa, t_1, t_2)} - u_d)^2 dx dt + \frac{\nu}{2} (t_1^2 + t_2^2 + \kappa^2).$$
(PS)

# 4.2 Discussion of (PG)

The control-to-state mapping G

Next, we discuss the differentiability of the control-to-state mappings  $g \mapsto u_g$  and  $(\kappa, t_1, t_2) \mapsto u(\kappa, t_1, t_2)$ . First, we consider the case of the general kernel g. The analysis for the particular kernel (6) is fairly analogous but cannot deduced as a particular case of (PG). We will briefly sketch it in a separate section.

By Theorem 1, we know that the mapping  $G: g \mapsto u_g$  is well defined from  $L^{\infty}(0,T)$  to  $C(\bar{Q})$ . Now we discuss the differentiability of G. To slightly simplify the notation, we introduce an operator  $\mathcal{K}: L^{\infty}(0,T) \times C(\bar{Q}) \to C(\bar{Q})$  by

$$\mathcal{K}(g, u) = K(g)u,$$

where K(g) was introduced in (9); notice that  $\mathcal{K}$  is bilinear. Let us first show the differentiability for  $\mathcal{K}$ .

We fix  $g \in L^{\infty}(0,T)$ ,  $u \in C(\bar{Q})$ , and select varying increments  $h \in L^{\infty}(0,T)$ ,  $v \in C(\bar{Q})$ . Then we have

$$\begin{split} \mathcal{K}(g+h,u+v) &= \int_0^T [g(\tau)+h(\tau)][u(x,t-\tau)+v(x,t-\tau)] \, d\tau \\ &= \int_0^t g(\tau)u(x,t-\tau) \, d\tau + \underbrace{\int_0^t h(\tau)u(x,t-\tau) \, d\tau + \int_0^t g(\tau)v(x,t-\tau) \, d\tau}_{A(g,u)(h,v)} \\ &+ \underbrace{\int_0^t h(\tau)v(x,t-\tau) \, d\tau}_{R(h,v)} &= \mathcal{K}(g,u) + A(g,u)(h,v) + R(h,v), \end{split}$$

where  $A(g,u): L^{\infty}(0,T) \times C(\bar{Q}) \to C(\bar{Q})$  is a linear continuous operator and  $R: L^{\infty}(0,T) \times C(\bar{Q}) \to C(\bar{Q})$  is a remainder term. It is easy to confirm that

$$\frac{\|R(h,v)\|_{C(\bar{Q})}}{\|(h,v)\|_{L^{\infty}(0,T)\times C(\bar{Q})}}\to 0, \quad \text{ if } \|(h,v)\|_{L^{\infty}(0,T)\times C(\bar{Q})}\to 0.$$

Therefore,  $\mathcal{K}$  is Fréchet-differentiable. As a continuous bilinear form,  $\mathcal{K}$  is also of class  $C^2$ .

Now, we investigate the control-to-state mapping  $G: L^{\infty}(0,T) \to C(\bar{Q})$  defined by  $G: g \mapsto u_g$ , where the state function  $u_g$  is defined as the unique solution to

$$\partial_t u - \Delta u + R(u) + \kappa u = \kappa \mathcal{K}(g, u) + \kappa U_g \text{ in } Q$$

$$\partial_n u = 0 \text{ in } \Sigma$$

$$u(0) = u_0(0) \text{ in } \Omega.$$
(14)

In what follows, the initial function  $u_0$  will be kept fixed and is therefore not mentioned. Of course,  $U_g$ , G and some of the operators below depend on  $u_0$ ,

but we will not explicitly mention this dependence. To discuss G, we need known properties of the following auxiliary mapping  $\mathcal{G}: v \mapsto u$ , where

$$\begin{array}{ll} \partial_t u - \Delta u + R(u) + \kappa \, u = v & \text{in } Q \\ \partial_n u = 0 & \text{in } \varSigma \\ u(0) = u_0(0) & \text{in } \varOmega. \end{array}$$

This mapping  $\mathcal{G}$  is of class  $\mathcal{C}^2$  from  $L^p(Q)$  to  $W(0,T) \cap \mathcal{C}(\bar{Q})$ , if  $p > \frac{5}{2}$ , in particular from  $L^{\infty}(Q)$  to  $L^{\infty}(Q)$ , cf. [8] or, for monotone R, [6], [24], [29].

Now (consider  $v := \kappa (\mathcal{K}(g, u) + U_g)$  as given and keep the initial function  $u_0$  fixed), u solves (14) if and only if  $u = \mathcal{G}(\kappa \mathcal{K}(g, u) + \kappa U_g)$ , i.e.

$$u - \mathcal{G}(\kappa \mathcal{K}(g, u) + \kappa U_g) = 0. \tag{15}$$

We introduce a new mapping  $\mathcal{F}: L^{\infty}(Q) \times L^{\infty}(0,T) \to L^{\infty}(Q)$  defined by

$$\mathcal{F}(u, g) := u - \mathcal{G}(\kappa \,\mathcal{K}(g, u) + \kappa \,U_g).$$

Then, (15) is equivalent to the equation

$$\mathcal{F}(u,g) = 0. \tag{16}$$

We have proved above that the mapping  $(g, u) \mapsto \mathcal{K}(g, u)$  is of class  $\mathcal{C}^2$  from  $L^{\infty}(0, T) \times L^{\infty}(Q)$  to  $L^{\infty}(Q)$ . Obviously, also the linear mapping  $g \mapsto U_g$  is of class  $\mathcal{C}^2$  from  $L^{\infty}(0, T)$  to  $L^{\infty}(Q)$ . By the chain rule, also  $\mathcal{F}$  is  $\mathcal{C}^2$  from  $L^{\infty}(Q) \times L^{\infty}(0, T) \to L^{\infty}(Q)$  and the mappings  $\partial_g \mathcal{F}(\bar{u}, \bar{g})$ ,  $\partial_u \mathcal{F}(\bar{u}, \bar{g})$  are continuous in the associated pairs of spaces.

To use the implicit function theorem, we prove that  $\partial_u \mathcal{F}(\bar{u}, \bar{g})$  is continuously invertible at any fixed pair  $(\bar{u}, \bar{g})$ . Therefore, we consider the equation

$$\partial_u \mathcal{F}(\bar{u}, \bar{g})v = z \tag{17}$$

with given right-hand side  $z \in L^{\infty}(Q)$  and show the existence of a unique solution  $v \in L^{\infty}(Q)$ . The equation is equivalent with

$$v - \mathcal{G}'(\underbrace{\kappa \mathcal{K}(\bar{g}, \bar{u}) + \kappa U_g}_{\bar{p}}) \kappa \mathcal{K}(g, v) = z.$$
(18)

Writing for convenience  $\bar{p} = \kappa \mathcal{K}(\bar{g}, \bar{u}) + \kappa U_g$ , we obtain the simpler form

$$v - \mathcal{G}'(\bar{p})\kappa K(\bar{q})v = z.$$

A function  $z \in L^{\infty}(Q)$  does not in general belong to W(0,T). To overcome this difficulty, we set w := v - z and transform the equation to

$$w = \mathcal{G}'(\bar{p}) \underbrace{\kappa K(\bar{g})(w+z)}_{q} = \mathcal{G}'(\bar{p})q. \tag{19}$$

where  $q := \kappa K(\bar{g})(w+z)$ . As the next result shows, w is the solution of a parabolic PDE, hence  $w \in W(0,T)$ .

**Lemma 1** Let  $q \in L^p(Q)$  with p > 5/2 be given. Then we have  $y = \mathcal{G}'(\bar{p})q$  if and only if y solves

$$\partial_t y - \Delta y + R'(\bar{u})y + \kappa y = q \text{ in } Q$$
  
 $\partial_n y = 0 \text{ in } \Sigma$   
 $y(0) = 0 \text{ in } \Omega,$ 

where  $\bar{u}$  is the solution associated with  $\bar{p}$ , i.e.

$$\begin{split} \partial_t \bar{u} - \Delta \bar{u} + R(\bar{u}) + \kappa \, \bar{u} &= \bar{p} \quad \text{in } Q \\ \partial_n \bar{u} &= 0 \quad \text{in } \Sigma \\ \bar{u}(0) &= u_0 \quad \text{in } \Omega. \end{split}$$

We refer to [8]. For monotone non-decreasing functions R, this result is well known in the theory of semilinear parabolic control problems, see e.g. [6], [23], or [29, Thm. 5.9]. By Lemma 1, the solution w of (19) is the unique solution of the linear PDE

$$(\partial_t w - \Delta w + R'(\bar{u})w + \kappa w)(x, t) = q(x, t)$$

$$= \kappa \int_0^t \bar{g}(\tau)w(x, t - \tau) d\tau + \kappa \int_0^t \bar{g}(\tau)z(x, t - \tau) d\tau$$
(20)

subject to w(0) = 0 and homogeneous Neumann boundary conditions. By the same methods as above we find that, for all  $z \in L^{\infty}(Q)$ , equation (20) has a unique solution  $w \in W(0,T) \cap L^{\infty}(Q)$ .

After transforming back by v = w + z, we have found that for all  $z \in L^{\infty}(Q)$ , (17) has a unique solution  $v \in L^{\infty}(Q)$  given by v = w + z. Therefore, the inverse operator  $\partial_u \mathcal{F}(\bar{u}, \bar{g})^{-1}$  exists. The continuity of this inverse mapping follows from a result of [8] that the mapping  $z \mapsto w$  defined by (20) is continuous in  $L^{\infty}(Q)$ .

Next, we consider the operator  $\partial_g \mathcal{F}$ . It exists by the chain rule and admits the form

$$\partial_g \mathcal{F}(\bar{u}, \bar{g})h = \mathcal{G}'(\kappa (K(\bar{g})\bar{u} + U_g))\kappa (K(h)\bar{u} + \partial_g U_g h).$$

Setting again  $\bar{p} = \kappa (K(\bar{g})\bar{u} + U_q)$  and  $q = \kappa (K(h)\bar{u} + \partial_q U_q h)$ , we see that

$$\partial_q \mathcal{F}(\bar{u}, \bar{g})h = \eta,$$

where, by Lemma 1,  $\eta$  solves the equation

$$\partial_t \eta - \Delta \eta + R'(\bar{u})\eta + \kappa \eta = q = \kappa K(h)\bar{u} + \kappa \partial_q U_q h$$

subject to homogeneous initial and boundary conditions. Therefore,  $\eta$  is the unique solution to

$$(\partial_t \eta - \Delta \eta + R'(\bar{u})\eta + \kappa \eta)(x, t) = \kappa \int_0^t h(\tau)\bar{u}(x, t - \tau) d\tau$$
$$+\kappa \int_t^T h(\tau)u_0(x, t - \tau) d\tau$$
$$\eta(x, 0) = 0$$
$$\partial_n \eta = 0.$$

By  $\bar{u}(x,t) = u_0(x,t)$  for  $-T \le t \le 0$ , we can re-write this as

$$(\partial_t \eta - \Delta \eta + R'(\bar{u})\eta + \kappa \eta)(x, t) = \kappa \int_0^T h(\tau)\bar{u}(x, t - \tau) d\tau$$
$$\partial_n \eta = 0$$
$$\eta(x, 0) = 0.$$

Again, the mapping  $h \mapsto w$  is continuous from  $L^{\infty}(0,T)$  to  $W(0,T) \cap \mathcal{C}(\bar{Q})$ .

Collecting the last results, we have the following theorem:

**Theorem 2 (Differentiability of** G) The control-to-state mapping  $G: g \mapsto u_g$  associated with equation (10) is of class  $C^2$ . The first order derivative z := G'(g)h is obtained as the unique solution to

$$(\partial_t z - \Delta z + R'(u_g)z + \kappa z)(x,t) = \kappa \int_0^T h(\tau)u_g(x,t-\tau) d\tau + \kappa \int_0^t g(\tau)z(x,t-\tau) d\tau \quad \text{in } Q$$

$$\partial_n z = 0 \quad \text{in } \Sigma$$

$$z(\cdot,t) = 0, \ -T \le t \le 0 \quad \text{in } \Omega.$$
(21)

*Proof* We already know by Theorem 1 that, for all  $g \in L^{\infty}(0,T)$ , there exists a unique solution  $u = G(g) \in W(0,T) \cap \mathcal{C}(\bar{Q})$  solving the equation

$$\mathcal{F}(u,g) = 0.$$

We have discussed above that the assumptions of the implicit function theorem are satisfied. Now this theorem yields that the mapping  $g \mapsto G(g)$  is of class  $C^2$ .

The derivative G'(g)h is obtained by implicit differentiation. By definition of G(g), we have

$$(\partial_t G(g) - \Delta G(g) + R(G(g)) + \kappa G(g))(x,t) = \kappa \int_0^t g(\tau) G(g)(x,t-\tau) d\tau$$
$$+\kappa \int_t^T g(\tau) u_0(x,t-\tau) d\tau$$
$$\partial_n G(g) = 0$$
$$G(g)(\cdot,t) = u_0(\cdot,t), \ -T \le t \le 0.$$
 (22)

Implicit differentiation yields that z := G'(g)h is the unique solution of (21). Notice that

$$\int_0^t g(\tau) \, G(g)(x,t-\tau) \, d\tau + \int_t^T g(\tau) \, u_0(x,t-\tau) \, d\tau = \int_0^T g(\tau) \, G(g)(x,t-\tau) \, d\tau.$$

# 4.3 Existence of an optimal kernel

**Theorem 3** For all  $\nu \geq 0$ , (PG) has at least one optimal solution  $\bar{g}$ .

Proof Let  $(g_n)$  with  $g_n \in C$  for all  $n \in \mathbb{N}$  be a minimizing sequence. Since C is bounded, convex, and closed in  $L^{\infty}(0,T)$ , we can assume without limitation of generality that  $g_n$  converges weakly in  $L^2(0,T)$  to  $\bar{g}$ , i.e.  $g_n \rightharpoonup \bar{g}$ ,  $n \to \infty$ . The associated sequence of states  $u_n$  obeys the equations

$$\partial_t u_n - \Delta u_n + \kappa u_n = d_n := -\kappa R(u_n) + \kappa K(g_n) u_n + \kappa U_g. \tag{23}$$

By the principle of superposition, we split the functions  $u_n$  as  $u_n = \hat{u} + \tilde{u}_n$ , where  $\hat{u}$  is the solution of (23) with right-hand side  $d_n := 0$  and initial value  $\hat{u}(0) = u_0(0)$ , while  $\tilde{u}_n$  is the solution to the right-hand side  $d_n$  defined above and zero initial value. In view of (13), all state functions  $u_n$ , hence also the functions  $\tilde{u}_n$ , are uniformly bounded in  $L^{\infty}(Q)$ . Thanks to [11, Thm. 4], the sequence  $(\tilde{u}_n)$  is bounded in some Hölder space  $C^{0,\lambda}(Q)$ . By the Arzela-Ascoli theorem, we can assume (selecting a subsequence, if necessary) that  $\tilde{u}_n$  converges strongly in  $L^{\infty}(Q)$ . Adding to  $\tilde{u}_n$  the fixed function  $\hat{u}$ , we have that  $(u_n)$  converges strongly to some  $\bar{u}$  in  $L^{\infty}(Q)$ .

The boundedness of  $(u_n)$  also induces the boundedness of the sequence  $(d_n)$  in  $L^{\infty}(Q)$ , in particular in  $L^2(Q)$ . Therefore, we can assume that  $d_n$  converges weakly in  $L^2(Q)$  to  $\bar{d}$ ,  $n \to \infty$ . Since  $(u_n)$  is the sequence of solutions to the "linear" equation (23) with right-hand side  $d_n$ , the weak convergence of  $(d_n)$  induces the weak convergence of  $u_n \to \bar{u}$  in W(0,T), where  $\bar{u}$  solves (23) with right-hand side  $\bar{d}$ .

Finally, we show that

$$\bar{d}(t) = -\kappa R(\bar{u}(t)) + \kappa \left( K(\bar{g})\bar{u} \right)(t) + \kappa U_q(t)$$

so that  $\bar{u}$  is the state associated with  $\bar{g}$ . Obviously, it suffices to prove that  $K(g_n)u_n$  converges weakly to  $K(\bar{g})\bar{u}$  in  $L^2(Q)$ . To this aim, let an arbitrary  $\varphi \in L^2(Q)$  be given. Then we have

$$\iint_{Q} \varphi(x,t) \left( \int_{0}^{t} g_{n}(\tau) u_{n}(x,t-\tau) d\tau \right) dx dt$$

$$= \int_{0}^{T} g_{n}(\tau) \left( \int_{\tau}^{T} \int_{\Omega} \varphi(x,t) u_{n}(x,t-\tau) dt dx \right) d\tau. \tag{24}$$

Clearly, the strong convergence of  $(u_n)$  in  $L^{\infty}(Q)$  yields

$$\int_{\tau}^{T} \int_{\Omega} \varphi(x,t) u_n(x,t-\cdot) dt dx \to \int_{\tau}^{T} \int_{\Omega} \varphi(x,t) \bar{u}(x,t-\cdot) dt dx$$

in  $L^2(0,T)$ . Along with the weak convergence of  $g_n$ , this implies

$$\lim_{n \to \infty} \int_0^T g_n(\tau) \int_{\tau}^T \int_{\Omega} \varphi(x, t) u_n(x, t - \tau) dt dx d\tau$$
$$= \int_0^T \bar{g}(\tau) \int_{\tau}^T \int_{\Omega} \varphi(x, t) \bar{u}(x, t - \tau) dt dx d\tau.$$

In view of (24), we finally arrive at

$$\iint_{Q} \varphi(x,t) \int_{0}^{t} g_{n}(\tau) u_{n}(x,t-\tau) \, d\tau dx dt \to \iint_{Q} \varphi(x,t) \int_{0}^{t} \bar{g}(\tau) \bar{u}(x,t-\tau) \, d\tau dx dt$$

as  $n \to \infty$ . Since this holds for arbitrary  $\varphi \in L^2(Q)$ , this is equivalent to the desired weak convergence  $K(g_n)u_n \to K(\bar{g})\bar{u}$  in  $L^2(Q)$ .

## 4.4 Necessary optimality conditions

#### 4.4.1 Adjoint equation

In the next step of our analysis, we establish the necessary optimality conditions for a (local) solution  $\bar{g}$  of the optimization problem (PG). This optimization problem is defined by

$$\begin{cases}
\min J(g), \\
0 \le g(t) \le \beta & \text{for almost all } t \in [0, T], \\
\int_0^T g(\tau) d\tau = 1.
\end{cases}$$
(25)

Although the admissible set belongs to  $L^{\infty}(0,T)$ , we consider this as an optimization problem in the Hilbert space  $L^{2}(0,T)$ .

To set up associated necessary optimality conditions for an optimal solution of (25), we first determine a useful expression for the derivative of the objective functional J. We have

$$J(g) = \frac{1}{2} \iint_{Q} c_{Q} (u_{g} - u_{d})^{2} dx dt + \frac{\nu}{2} \int_{0}^{T} g(t)^{2} dt$$
$$= \frac{1}{2} \iint_{Q} c_{Q} (G(g) - u_{d})^{2} dx dt + \frac{\nu}{2} \int_{0}^{T} g(t)^{2} dt.$$

Let now be an arbitrary (i.e. not necessarily optimal)  $\bar{g} \in L^{\infty}(0,T)$  be given and let  $\bar{u} = G(\bar{g})$  be the associated state. Then we obtain for  $h \in L^{\infty}(0,T)$ 

$$J'(\bar{g})h = \nu \int_{0}^{T} \bar{g}(t) h(t) dt + \iint_{Q} c_{Q}(\bar{u} - u_{d}) (G'(\bar{u})h) dxdt$$
$$= \int_{0}^{T} \nu \bar{g}(t)h(t)dt + \iint_{Q} c_{Q}(x,t)(\bar{u}(x,t) - u_{d}(x,t))z(x,t)dxdt (26)$$

with the solution z to the equation (21) for  $u_g := u_{\bar{g}} = \bar{u}$ .

The implicit appearance of h via z can be converted to an explicit one by an *adjoint equation*. This is the following equation:

$$(-\partial_{t}\varphi - \Delta\varphi + R'(\bar{u})\varphi + \kappa\varphi)(x,t) = \kappa \int_{0}^{T} \bar{g}(\tau)\varphi(x,t+\tau) d\tau + c_{Q}(x,t)(\bar{u}(x,t) - u_{d}(x,t))$$
a.e. in  $Q$ ,
$$\partial_{n}\varphi = 0 \quad \text{in } \Sigma,$$

$$\varphi(\cdot,t) = 0 \quad t \in [T,2T].$$

$$(27)$$

The solution  $\bar{\varphi}$  of (27) is said to be the *adjoint state* associated with  $\bar{g}$ .

**Lemma 2** Let  $\bar{g}$ ,  $\bar{h} \in L^{\infty}(0,T)$ , and  $\bar{u} = u_{\bar{g}}$  be given. If z is the solution to the linearized equation (21) for  $u_g := \bar{u}$  and  $\bar{\varphi}$  is the unique solution to the adjoint equation (27), then the identity

$$\iint_{Q} (c_{Q}(\bar{u} - u_{d})z)(x,t) dxdt = \kappa \iint_{Q} \bar{\varphi}(x,t) \left( \int_{0}^{T} h(\tau)\bar{u}(x,t-\tau) d\tau \right) dxdt$$
(28)

is fulfilled:

*Proof* We multiply the first equation in (21) by the adjoint state  $\bar{\varphi}$  as test function and the first equation in (27) by z. After integration on Q and some partial integration with respect to x, we obtain

$$\iint_{Q} (\partial_{t}z\,\bar{\varphi} + \nabla z \cdot \nabla \bar{\varphi} + (R'(\bar{u}) + \kappa)z\,\bar{\varphi})\,dxdt$$

$$= \kappa \iint_{Q} \left( \int_{0}^{T} \bar{g}(\tau)z(x, t - \tau)\,d\tau \right) \bar{\varphi}(x, t)\,dxdt$$

$$+ \kappa \iint_{Q} \left( \int_{0}^{T} h(\tau)\bar{u}(x, t - \tau)\,d\tau \right) \bar{\varphi}(x, t)\,dxdt$$

and

$$\iint_{Q} (-z \,\partial_{t} \bar{\varphi} + \nabla z \cdot \nabla \bar{\varphi} + (R'(\bar{u}) + \kappa)z \,\bar{\varphi}) \,dxdt$$

$$= \kappa \iint_{Q} \left( \int_{0}^{T} \bar{g}(\tau) \bar{\varphi}(x, t + \tau) \,d\tau \right) z(x, t) \,dxdt + \iint_{Q} c_{Q}(\bar{u} - u_{d}) \,z \,dxdt.$$

Integrating by parts with respect to t, we see that

$$\iint_{Q} (-z) \, \partial_t \bar{\varphi} \, dx dt = \iint_{Q} \bar{\varphi} \, \partial_t z \, dx dt;$$

notice that we have z(0) = 0 and  $\bar{\varphi}(T) = 0$ . Comparing both weak formulations above, it turns out that we only have to confirm the equation

$$\iint_{Q} \int_{0}^{T} \bar{g}(\tau) z(x, t - \tau) \, \bar{\varphi}(x, t) \, d\tau \, dx dt = \iint_{Q} \int_{0}^{T} \bar{g}(\tau) \bar{\varphi}(x, t + \tau) \, z(x, t) \, d\tau \, dx dt.$$
(29)

Then the claim of the Lemma follows. To show (29) , we proceed as follows:

$$\iint_{Q} \int_{0}^{T} \bar{g}(\tau)z(x,t-\tau)\varphi(x,t) d\tau dxdt 
= \int_{\Omega} \int_{0}^{T} \int_{0}^{T} \bar{g}(\tau)z(x,t-\tau)\bar{\varphi}(x,t) d\tau dtdx 
= \int_{\Omega} \int_{0}^{T} \int_{0}^{t} \bar{g}(\tau)z(x,t-\tau)\bar{\varphi}(x,t) d\tau dtdx 
= \int_{\Omega} \int_{0}^{T} \int_{0}^{t} \bar{g}(t-\eta)z(x,\eta)\bar{\varphi}(x,t) d\eta dt dx 
= \int_{\Omega} \int_{0}^{T} \int_{\eta}^{T} \bar{g}(t-\eta)\bar{\varphi}(x,t) dt z(x,\eta) d\eta dx 
= \int_{\Omega} \int_{0}^{T} \int_{0}^{T-\eta} \bar{g}(\sigma)\bar{\varphi}(x,\eta+\sigma) d\sigma z(x,\eta) d\eta dx 
= \int_{\Omega} \int_{0}^{T} \int_{0}^{T} \bar{g}(\sigma)\bar{\varphi}(x,\eta+\sigma) d\sigma z(x,\eta) d\eta dx 
= \iint_{\Omega} \int_{0}^{T} \bar{g}(\tau)\bar{\varphi}(x,t+\tau)z(x,t) d\tau dxdt.$$
(30)

We used  $z(x, t - \tau) = 0$  for  $\tau > t$  (due to (21)) in the second equation, the substitution  $\eta = t - \tau$  in the third, the Fubini theorem in the fourth, the substitution  $\sigma = t - \eta$  in the fifth, the property  $\bar{\varphi}(x, t) = 0$  for  $t \geq T$  in the sixth equation. Finally, we re-named the variables.

**Corollary 1** At any  $\bar{g} \in L^{\infty}(0,T)$ , the derivative  $J'(\bar{g})h$  in the direction  $h \in L^{\infty}(0,T)$  is given by

$$J'(\bar{g}) h = \int_0^T \nu \,\bar{g}(t) \,h(t) \,dt + \kappa \int_0^T h(\tau) \left( \iint_Q \bar{\varphi}(x,t) \bar{u}(x,t-\tau) \,dx dt \right) d\tau,$$

where  $\bar{\varphi}$  is the unique solution of the adjoint equation (27).

This follows immediately by inserting the right-hand side of (28) in (26) and by interchanging the order of integration with respect to t and  $\tau$ .

# 4.4.2 Necessary optimality conditions for (PG)

Let us now establish the necessary optimality conditions for an optimal solution  $\bar{g}$  of (25). They can be derived by the Lagrangian function  $L: L^{\infty}(0,T) \times \mathbb{R} \to \mathbb{R}$ ,

$$L(g,\mu) := J(g) + \mu \left( \int_0^T g(\tau) \, d\tau - 1 \right).$$

If  $\bar{g}$  is an optimal solution, then there exists a real Lagrange multiplier  $\bar{\mu}$  such that the variational inequality

$$J'(\bar{g})(g-\bar{g}) + \bar{\mu} \int_0^T (g-\bar{g}) dt \ge 0 \qquad \text{for all } g \ge 0$$

is satisfied. Inserting the result of Corollary 1 for  $h := g - \bar{g}$ , we find

$$\int_0^T \left(\nu \bar{g}(t) + \bar{\mu} + \kappa \iint_Q \bar{\varphi}(x, s) \bar{u}(x, s - t) \, dx ds\right) \left(g(t) - \bar{g}(t)\right) dt \ge 0 \quad (31)$$

for all  $0 \le g \le \beta$ .

Remark 2 For a Lagrange multiplier rule to hold, a regularity condition must be fulfilled. Here, the constraints are obviously regular at any  $\bar{g}$ : Define  $F: L^2(0,T) \to \mathbb{R}$  by

$$F(g) = \int_0^T g(\tau) d\tau - 1.$$

Then

$$F'(g)h = \int_0^T h(\tau) d\tau,$$

and hence  $F'(g): L^2(0,T) \to \mathbb{R}$  is surjective for all  $g \in L^2(0,T)$ .

A simple pointwise discussion of (31) leads to the following complementarity conditions for almost all  $t \in [0, T]$ :

$$g(t) = \begin{cases} 0 \text{ if } \nu \bar{g}(t) + \bar{\mu} + \kappa \iint_{Q} \bar{\varphi}(x,s)\bar{u}(x,s-t) \, dx ds > 0 \\ \beta \text{ if } \nu \bar{g}(t) + \bar{\mu} + \kappa \iint_{Q} \bar{\varphi}(x,s)\bar{u}(x,s-t) \, dx ds < 0. \end{cases}$$
(32)

If the expression in right-hand side above vanishes, then we obviously have

$$g(t) = -\frac{1}{\nu} \left( \bar{\mu} + \kappa \iint_{Q} \bar{\varphi}(x, s) \bar{u}(x, s - t) \, dx ds \right).$$

In a known way, the last three relations can be equivalently expressed by the projection formula

$$\bar{g}(t) = \mathbb{P}_{[0,\beta]} \left( -\frac{1}{\nu} \left( \bar{\mu} + \kappa \iint_{Q} \bar{\varphi}(s) \bar{u}(x,s-t) \, dx ds \right) \right),$$

where  $\mathbb{P}_{[0,\beta]}: \mathbb{R} \to [0,\beta]$  is defined by

$$\mathbb{P}_{[0,\beta]}(x) = \max(0, \min(\beta, x)).$$

## 5 Discussion of (PS)

Let us now discuss the changes that are needed to establish the necessary optimality conditions for the problem (PS) with the particular form (6) of g. Now,  $\kappa, t_1$ , and  $t_2$  are our control variables. Let us denote by  $u_{(\kappa, t_1, t_2)}$  the unique state associated with  $(\kappa, t_1, t_2)$ .

The existence of the derivatives  $\partial_{t_i} u_{(\kappa,t_1,t_2)}$ , i=1,2, and  $\partial_{\kappa} u_{(\kappa,t_1,t_2)}$  can be shown again by the implicit function theorem. We omit these details, because one can proceed analogously to the discussion for (PG). To shorten the notation, we write

$$z_i := \partial_{t_i} u_{(\kappa, t_1, t_2)}, \ i = 1, 2, \quad z_3 := \partial_{\kappa} u_{(\kappa, t_1, t_2)}.$$

By implicit differentiation, we find the functions  $z_i$  from linearized equations. Assume that the derivatives have to be determined at the point  $(\kappa, t_1, t_2)$  and fix the associated state  $u := u_{(\kappa, t_1, t_2)}$  for a while. Then,  $z_1$  solves

$$(\partial_t z_1 - \Delta z_1 + R'(u)z_1 + \kappa z_1)(x,t) = \frac{\partial}{\partial t_1} \left[ \frac{\kappa}{t_2 - t_1} \int_{t_1}^{t_2} u(x,t-\tau) d\tau \right]$$

$$= \frac{\kappa}{t_2 - t_1} \left[ \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} u(x,t-\tau) d\tau - u(x,t-t_1) + \int_{t_1}^{t_2} z_1(x,t-\tau) d\tau \right].$$
(33)

Analogously, we find for  $z_2$ 

$$(\partial_t z_2 - \Delta z_2 + R'(u)z_2 + \kappa z_2)(x,t) =$$

$$= \frac{-\kappa}{t_2 - t_1} \left[ \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} u(x,t-\tau) d\tau - u(x,t-t_2) + \int_{t_1}^{t_2} z_2(x,t-\tau) d\tau \right]$$
(34)

and for  $z_3$ 

$$(\partial_t z_3 - \Delta z_3 + R'(u)z_3 + \kappa z_3 + u)(x,t) = \frac{\partial}{\partial \kappa} \left[ \frac{\kappa}{t_2 - t_1} \int_{t_1}^{t_2} u(x,t-\tau) d\tau \right]$$
$$= \frac{1}{t_2 - t_1} \left[ \int_{t_1}^{t_2} u(x,t-\tau) d\tau + \kappa \int_{t_1}^{t_2} z_3(x,t-\tau) d\tau \right].$$

Therefore, the equation for  $z_3$  is

$$(\partial_t z_3 - \Delta z_3 + R'(u)z_3 + \kappa z_3)(x,t) - \frac{\kappa}{t_2 - t_1} \int_{t_1}^{t_2} z_3(x,t-\tau) d\tau$$

$$= \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} u(x,t-\tau) d\tau - u(x,t).$$
(35)

Again, we introduce an adjoint equation to set up the optimality conditions. To this aim, let  $(\kappa, t_1, t_2)$  an arbitrary fixed triplet and  $u_{(\kappa, t_1, t_2)}$  be the associated

state function. The adjoint equation is

$$(-\varphi_t - \Delta \varphi + R'(u_{(\kappa,t_1,t_2)})\varphi + \kappa \varphi) (x,t) = \frac{\kappa}{t_2 - t_1} \int_{t_1}^{t_2} \varphi(x,t+\tau) d\tau + c_Q(x,t) (u_{(\kappa,t_1,t_2)}(x,t) - u_d(x,t))$$
in  $Q$ ,
$$\partial_n \varphi = 0 \quad \text{in } \Sigma,$$

$$\varphi(x,t) = 0 \quad \text{in } \Omega \times [T,2T].$$

$$(36)$$

This equation has a unique solution  $\varphi \in L^{\infty}(Q)$  denoted by  $\varphi_{(\kappa,t_1,t_2)}$  to indicate the correspondence with  $(\kappa,t_1,t_2)$ . Existence and uniqueness can be shown in a standard way by the substitution  $\tilde{t} := T - t$  that transforms this equation to a standard forward equation that can be handled in the same way as the state equation.

**Theorem 4 (Derivative of**  $J_S$ ) Let  $(\kappa, t_1, t_2)$  be given,  $u := u_{(\kappa, t_1, t_2)}$  be the associated state, and  $\varphi := \varphi_{(\kappa, t_1, t_2)}$  be the associated adjoint state, i.e. the unique solution of the adjoint equation (36). Write for short  $\delta := 1/(t_2 - t_1)$ . Then the partial derivatives of  $J_S$  at  $(\kappa, t_1, t_2)$  are given by

$$\partial_{t_1} J_S = \nu t_1 + \frac{\kappa}{\delta} \iint_Q \varphi(x, t) \left[ \frac{1}{\delta} \int_{t_1}^{t_2} u(x, t - \tau) d\tau - u(x, t - t_1) \right] dx dt,$$

$$\partial_{t_2} J_S = \nu t_2 - \frac{\kappa}{\delta} \iint_Q \varphi(x, t) \left[ \frac{1}{\delta} \int_{t_1}^{t_2} u(x, t - \tau) d\tau - u(x, t - t_2) \right] dx dt$$

$$\partial_{\kappa} J_S = \nu \kappa + \iint_Q \varphi(x, t) \left[ \frac{1}{\delta} \int_{t_1}^{t_2} u(x, t - \tau) d\tau - u(x, t) \right] dx dt.$$

Proof We verify the expression for  $\partial_{t_1} J_S(\kappa, t_1, t_2)$ , the other formulas can be shown analogously. To this aim, let  $z_1 = \partial_{t_1} u_{(\kappa, t_1, t_2)}$  be the solution of the linearized equation (33). For convenience, we write  $z := z_1$  within this proof. Following the proof of Lemma 2, we multiply (33) by  $\varphi$  and integrate over Q. We obtain

$$\iint_{Q} (\partial_{t}z \varphi + \nabla z \cdot \nabla \varphi + (R'(u) + \kappa)z \varphi) dxdt$$

$$= \frac{\kappa}{\delta} \iint_{Q} \varphi(x,t) \left[ \frac{1}{\delta} \int_{t_{1}}^{t_{2}} u(x,t-\tau) d\tau - u(x,t-t_{1}) \right] dxdt \qquad (37)$$

$$+ \frac{\kappa}{\delta} \iint_{Q} \varphi(x,t) \int_{t_{1}}^{t_{2}} z(x,t-\tau) d\tau dxdt.$$

Next, we multiply the adjoint equation (36) by z and integrate over Q to find

$$\iint_{Q} (-z \,\partial_{t} \varphi + \nabla z \cdot \nabla \varphi + (R'(u) + \kappa)z \,\varphi) \,dxdt$$

$$= \frac{\kappa}{\delta} \iint_{Q} \int_{t_{1}}^{t_{2}} \varphi(x, t + \tau) \,d\tau \,z(x, t) \,dxdt + \iint_{Q} c_{Q}(\bar{u} - u_{d}) \,z \,dxdt.$$
(38)

Now recall that

$$g(t) = \begin{cases} \frac{1}{t_2 - t_1}, t_1 \le t \le t_2\\ 0, & \text{elsewhere.} \end{cases}$$

Therefore, we can write

$$\begin{split} &\frac{1}{\delta} \iint_{Q} \varphi(x,t) \int_{t_{1}}^{t_{2}} z(x,t-\tau) \, d\tau dx dt = \iint_{Q} \int_{0}^{T} \varphi(x,t) g(\tau) z(x,t-\tau) \, d\tau dx dt \\ &= \iint_{Q} \int_{0}^{T} g(\tau) \varphi(x,t+\tau) d\tau z(x,t) dx dt = \frac{1}{\delta} \iint_{Q} \int_{t_{1}}^{t_{2}} \varphi(x,t+\tau) d\tau z(x,t) dx dt, \end{split}$$

where the second equation follows from (30). In view of

$$\iint_{Q} (-z) \,\partial_t \varphi \, dx dt = \iint_{Q} \varphi \, \partial_t z \, dx dt,$$

a comparison of the equations (37) and (38) yields

$$\iint_{Q} c_{Q}(u - u_{d}) z \, dx dt =$$

$$= \frac{\kappa}{\delta} \iint_{Q} \varphi(x, t) \left[ \frac{1}{\delta} \int_{t_{1}}^{t_{2}} u(x, t - \tau) \, d\tau - u(x, t - t_{1}) \right] dx dt.$$

Since

$$\partial_{t_1} \left[ \frac{1}{2} \iint_Q c_Q (u_{(\kappa, t_1, t_2)} - u_d)^2 dx dt \right] = \iint_Q c_Q (u_{(\kappa, t_1, t_2)} - u_d) \, z_1 \, dx dt,$$

the first claim of the theorem follows immediately.

As a direct consequence of the theorem on the derivative of  $J_S$ , we obtain the following corollary.

Corollary 2 (Necessary optimality condition for (PS)) Let  $(\bar{\kappa}, \bar{t}_1, \bar{t}_2)$  be optimal for the problem (PS) and let  $\bar{u} := u_{(\bar{\kappa}, \bar{t}_1, \bar{t}_2)}$  and  $\bar{\varphi} := \varphi_{(\bar{\kappa}, \bar{t}_1, \bar{t}_2)}$  denote the associated state and adjoint state, respectively. Then, with the gradient  $\nabla J_S(\bar{\kappa}, \bar{t}_1, \bar{t}_2)$  defined by Theorem 4 with  $\bar{\varphi}$  and  $\bar{u}$  inserted for  $\varphi$  and u, respectively, the variational inequality

$$\nabla J_S(\bar{\kappa}, \bar{t}_1, \bar{t}_2) \cdot (\kappa - \bar{\kappa}, t_1 - \bar{t}_1, t_2 - \bar{t}_2)^{\top} \ge 0 \quad \forall (\kappa, t_1, t_2) \in C_{\delta}$$
 (39)

is satisfied.

Since the variable  $\kappa$  is unrestricted, the associated part of the variational inequality amounts to

$$\nu\bar{\kappa} - \iint_Q \bar{\varphi}(x,t)\bar{u}(x,t)\,dxdt + \frac{1}{\bar{t}_2 - \bar{t}_1}\iint_Q \bar{\varphi}(x,t)\bar{u}(x,t - \bar{t}_2)\,dxdt = 0.$$

If  $(\bar{t}_1, \bar{t}_2)$  belongs to the interior of the admissible set  $C_{\delta}$ , then the associated components of  $\nabla J_S$  must vanish as well, hence

$$\begin{split} \nu \bar{t}_1 + \frac{\bar{\kappa}}{\bar{t}_2 - \bar{t}_1} \iint_Q \bar{\varphi}(x,t) \left[ \frac{1}{\bar{t}_2 - \bar{t}_1} \int_{\bar{t}_1}^{\bar{t}_2} \bar{u}(x,t-\tau) \, d\tau - \bar{u}(x,t-\bar{t}_1) \right] \, dx dt &= 0 \\ \nu \bar{t}_2 - \frac{\bar{\kappa}}{\bar{t}_2 - \bar{t}_1} \iint_Q \bar{\varphi}(x,t) \left[ \frac{1}{\bar{t}_2 - \bar{t}_1} \int_{\bar{t}_2}^{\bar{t}_2} \bar{u}(x,t-\tau) \, d\tau - \bar{u}(x,t-\bar{t}_2) \right] \, dx dt &= 0. \end{split}$$

Remark 3 (Application of the formal Lagrange technique) To find the form of  $\nabla J_S$  and for establishing the necessary optimality conditions, it might be easier to apply the following standard technique that is slightly formal but leads to the same result: We set up the Lagrangian function  $\mathcal{L}$ ,

$$\mathcal{L}(u, \kappa, t_1, t_2, \varphi) = \frac{1}{2} \iint_Q c_Q(u - u_d)^2 dx dt - \iint_Q \varphi(x, t) \cdot \left[ (\partial_t u - \Delta u + R(u) + \kappa u)(x, t) - \frac{\kappa}{t_2 - t_1} \int_{t_1}^{t_2} u(x, t - \tau) d\tau \right] dx dt.$$

If  $(\kappa, t_1, t_2)$  is a given triplet, then the adjoint equation for the adjoint state  $\varphi_{(\kappa, t_1, t_2)}$  is found by

$$\partial_{u}\mathcal{L}(u,\kappa,t_{1},t_{2},\varphi) v = 0 \quad \forall v : v(\cdot,t) = 0 \text{ for } t \leq 0.$$

The derivatives of  $J_S$  are obtained by associated derivatives of  $\mathcal{L}$ . For instance, we have

$$\partial_t J_S(\kappa, t_1, t_2) = \partial_t \mathcal{L}(u, \kappa, t_1, t_2, \varphi)$$

if  $u = u_{(\kappa,t_1,t_2)}$  and  $\varphi = \varphi_{(\kappa,t_1,t_2)}$  are inserted after having taken the derivative of  $\mathcal{L}$  with respect to  $t_i$ . This obviously yields the first two components of  $\nabla J_S$  in Theorem 4. For the third component, we proceed analogously.

#### 6 Numerical examples for (PS)

#### 6.1 Introductory remarks

The numerical solution of the problems posed above requires techniques that are adapted to the desired type of patterns  $u_d$ . In this paper, we concentrate on numerical examples for the simplified problem (PS), where the kernel g is a step function. Although this problem is mathematically equivalent to a nonlinear optimization problem in a convex admissible set of  $\mathbb{R}^3$ , the obtained patterns are fairly rich and interesting in their own. In a forthcoming paper

to be published elsewhere, we will report on the numerical treatment of the more general problem (PG), where a kernel function g is to be determined.

In this section, we present some results for the problem (PS), where a standard regularized tracking type functional J is to be minimized in the set  $C_{\delta}$ . It will turn out that (PS) is only suitable for tracking desired states  $u_d$  of simple structure. In all what follows,  $\Omega = (a, b)$  is an open interval, i.e. we concentrate on the spatially one-dimensional case.

Compared to many optimal control problems for semilinear parabolic equations that were investigated in the literature, the numerical solution of the problems posed here is a bit delicate. We are interested in approximating desired states  $u_d$  that exhibit certain geometrical patterns. If they have a periodic structure, then the objective function J may exhibit many local minima with very narrow regions of attraction for the convergence of numerical techniques. Therefore, the optimization methods should be started in a sufficiently small neighborhood around the desired optimal solution. Moreover, the standard functional J does not really fit to our needs. We will address the tracking of periodic patterns  $u_d$  in Section 7.

#### 6.2 Discretization of the feedback system

To discretize the feedback equation (6), we apply an implicit Euler scheme with respect to the time and a finite element approximation by standard piecewise linear and continuous ansatz functions ("hat functions") with respect to the space variable.

For this purpose, we define a time grid by an equidistant partition of [0,T] with mesh size  $\tau = T/m$  and node points  $t_j = j\,\tau$ ,  $j = 0,\ldots,m$ . Associated with this time grid, functions  $u_j:\Omega\to\mathbb{R}$  are to be computed that approximate  $u(\cdot,t_j),\ j=0,\ldots,m$ , i.e.  $u_j\sim u(\cdot,t_j)$ . Based on the functions  $u_j$ , we define grid functions  $u^\tau:Q\to\mathbb{R}$  by piecewise linear approximation,

$$u^{\tau}(x,t) = \frac{1}{\tau}[(t_{j+1}-t)u_j(x) + (t_j-t)u_{j+1}(x)], \text{ if } t \in [t_j,t_{j+1}], \ j=0,\ldots,m.$$

By the implicit Euler scheme, the following system of nonlinear equations is set up,

$$\frac{u^{\tau}(x,t_{j+1}) - u^{\tau}(x,t_{j})}{\tau} - \Delta u^{\tau}(x,t_{j+1}) + R(u^{\tau}(x,t_{j+1}))$$

$$= \frac{\kappa}{t_{2} - t_{1}} \int_{t_{1}}^{t_{2}} u^{\tau}(x,t_{j+1} - s) ds - \kappa u^{\tau}(x,t_{j+1}), \quad j = 0,\dots, m - 1.$$

The spatial approximation is based on an equidistant partition of  $\Omega = (a, b)$  with mesh size h > 0. Here, we define standard piecewise affine and continuous ansatz functions (hat functions)  $\phi_i : \Omega \to \mathbb{R}$  and approximate the grid function  $u^{\tau}$  by  $u_h^{\tau}$ ,

$$u_h^{\tau}(x, t_j) = \sum_{i=0}^n u_{ji} \phi_i(x)$$

with unknown coefficients  $u_{ji} \in \mathbb{R}$ , j = 0, ..., m, i = 0, ..., n.

To set up the discrete system, we define vectors  $\mathbf{u}^j \in \mathbb{R}^{n+1}$  by  $\mathbf{u}^j = (u_{j0}, \dots, u_{jn})^\top$ ,  $j = 0, \dots, m$ . Moreover, we establish the mass and stiffness matrices

$$M := \left( \int_{\Omega} \phi_k(x) \phi_\ell(x) \, dx \right)_{k,\ell=0}^n, \quad A := \left( \int_{\Omega} \phi_k'(x) \phi_\ell'(x) \, dx \right)_{k,\ell=0}^n,$$

and, for j = 0, ..., m, the vectors

$$\begin{split} R(\mathbf{u}^j) &:= \left(\int_{\varOmega} R(u_h^\tau(x,t_j)) \, \phi_i(x) \, dx\right)_{i=0}^n \\ K(\mathbf{u}^j) &:= \frac{\kappa}{t_2 - t_1} \left(\int_{\varOmega} \int_{t_1}^{t_2} (u_h^\tau(x,t_j) - s) \, ds \, \phi_i(x) \, dx\right)_{i=0}^n. \end{split}$$

Remark 4 To compute the integrals  $R(\mathbf{u}^j)$ , we invoke a 4 point Gauss integration. Notice that the functions  $x \mapsto R(u_h^{\tau}(x,t_j))$  are third order polynomials so that the integrand of  $R(\mathbf{u}^j)$  is a polynomial of order 4. Here, the 4 point Gauss integration is exact.

For the computation of the vectors  $K(\mathbf{u}^j)$ , we use the trapezoidal rule. Here, for  $t_j - s \leq 0$ , the values  $u_0(x, t_j - s)$  must be inserted. To increase the precision, the primitive of  $u_0$  is used. The complete discrete system is

$$M\mathbf{u}^{j+1} - M\mathbf{u}^{j} + \tau A\mathbf{u}^{j+1} + \tau R(\mathbf{u}^{j+1}) = \tau K(\mathbf{u}^{j+1}) - \tau \kappa M\mathbf{u}^{j+1}$$
  $j = 0, 1, \dots m-1$ .

We define

$$F(\mathbf{u}) := [(1 + \tau \kappa)M + \tau A]\mathbf{u} + \tau R(\mathbf{u}) - \tau K(\mathbf{u}).$$

In each time step, we solve the nonlinear equation  $F(\mathbf{u}) = M\mathbf{u}^j$  to obtain  $\mathbf{u}^{j+1}$ . To this aim, we apply a fixed point iteration.

#### 6.3 Numerical examples for the standard tracking functional

For testing our numerical method, we generate the desired state  $u_d$  as solution of the feedback system for a given triplet  $(\hat{\kappa}, \hat{t}_1, \hat{t}_2)$ , i.e.

$$u_d := u_{(\hat{\kappa}, \hat{t}_1, \hat{t}_2)}.$$

If the regularization parameter  $\nu$  is small, then the numerical solution of (PS) should return a vector that is close to  $(\hat{\kappa}, \hat{t}_1, \hat{t}_2)$ .

In all of our computational examples, we selected a small number  $\delta > 0$  so that the restriction  $t_2 - t_1 \ge \delta$  was never active. Moreover, the Tikhonov regularization parameter  $\nu$  was set to zero, because a regularization was not needed for having numerical stability. This indicates that the unknown locally optimal solution satisfies a second-order sufficient optimality condition, since this is known to be sufficient for numerical stability of the solution. In this case, one should also be able to show that, for  $\nu \downarrow 0$ , the sequence of associated

(locally) optimal solutions tends to the solution for  $\nu = 0$ . We do not discuss this fairly technical issue here.

In the first numerical examples of this paragraph, the aim is to generate desired wave type solutions that expand with a given velocity.

Example 1 (Desired traveling wave with pre-computed  $u_d$ ) We select  $\Omega = (-20, 20)$ , T = 40,  $u_1 = 0$ ,  $u_2 = 0.25$ ,  $u_3 = 1$ ,  $\kappa = 0.5$ . Moreover, we take as initial function

$$u_0(x,t) := \frac{1}{2} \left( 1 - \tanh\left(\frac{x - vt}{2\sqrt{2}}\right) \right), \quad x \in \Omega, t \le 0,$$

where  $v = (1-2u_2)/\sqrt{2}$  is the velocity of the uncontrolled traveling wave given by  $u_0$ . Following the strategy explained above, we fix the triplet  $(\hat{\kappa}, \hat{t}_1, \hat{t}_2)$  by (0.5, 0.456, 0.541) and obtain  $u_d = u_{(\hat{\kappa}, \hat{t}_1, \hat{t}_2)}$ . This is a traveling wave with a smaller velocity  $v_d \approx 0.25$  due to the control term. To test our method, we apply our optimization algorithm to find  $(\bar{\kappa}, \bar{t}_1, \bar{t}_2)$  such that the associated state function u coincides with  $u_d$ . The method should return a result  $(\kappa, t_1, t_2)$  that is close to the vector (0.5, 0.456, 0.541).

To solve the problem (PS) in Example 1, we applied the MATLAB code fmincon. For the gradient  $\nabla J_S(\kappa, t_1, t_2)$ , a subroutine was implemented by our adjoint calculus. In this way, we were able to use the differentiable mode of fmincon.

During the optimization, we fixed  $\kappa = 0.5$  and considered the minimization only with respect to  $(t_1, t_2)$ . Taking  $t_1 = 0$ ,  $t_2 = 1$  as initial iterate for the optimization, fmincon returned  $t_1 = 0.4322$ ,  $t_2 = 0.5649$  as solution; notice that we fixed  $\nu = 0$ . The computed optimal value was  $J_S(\kappa, t_1, t_2) = 3.305e - 06$  and the Euclidean norm of the gradient was  $\|\nabla J_S(\kappa, t_1, t_2)\| = 4.194e - 03$ . The result is displayed in Fig. 1.

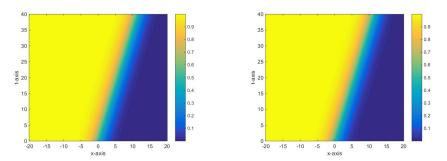


Fig. 1 Example 1, desired traveling wave  $u_d$  (left) and computed optimal state u (right).

Example 2 (Stopping a traveling wave) In contrast to Example 1, here we fix the desired pattern  $u_d$  that is displayed in Fig. 2, left side. This desired pattern was not pre-computed but geometrically designed, i.e. it is a "synthetic"

pattern that shows a traveling wave stopping at the time  $t \approx 16$ . The other data are selected as in Example 1.

In the optimization process for Example 2, we fixed  $\kappa = -1.5$ . The initial iterate was  $t_1 = 0$ ,  $t_2 = 1$ ; fmincon returned  $t_1 = 0.05$ ,  $t_2 = 0.94$  as solution. The optimal state is displayed in Fig. 2.

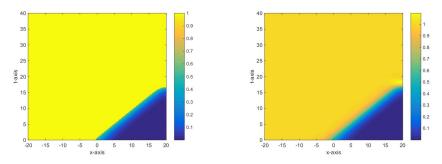


Fig. 2 Example 2, synthetic desired state  $u_d$  (left) and computed optimal state u (right).

The next example shows that the applicability of the standard tracking functional J of (PS) is limited to simple patterns  $u_d$ , e.g. wave type solutions of constant velocity.

Example 3 (Periodic pattern) Also here,  $u_d$  is a synthetic pattern that was not precomputed. In  $\Omega = (-20, 20)$ , we define

$$u_d(x,t) = 3\sin(t - \cos(\frac{\pi}{40}(x+40))).$$

Notice that this function  $u_d$  obeys the homogeneous Neumann boundary conditions. It is displayed in Fig. 3, left. Since such a periodic pattern cannot be expected for small times, we consider the tracking only on [T/2, T]. Therefore, here we re-define the objective functional J by

$$J_S(\kappa, t_1, t_2) := \int_{T/2}^T \int_{\Omega} (u_{(\kappa, t_1, t_2)} - u_d)^2 \, dx dt + \frac{\nu}{2} (\kappa^2 + t_1^2 + t_2^2).$$

During the optimization run, we fixed the values  $\kappa = -2$  and  $t_1 = 0$  and optimized only with respect to  $t_2$ . Starting from  $t_2 = 2$ , the code fmincon returned the solution  $t_2 = 3.7163$ . At this point, the Euclidean norm of  $\nabla J_S$  is  $|\nabla J_S(-2,0,3.7163)| \approx 0.0451$ . This is a fairly good value and indicates that the result should be close to a local minimum. Nevertheless, the computed optimal objective value is very large,

$$J_S(-2, 0, 3.7163) = 1.322 \cdot 10^3.$$

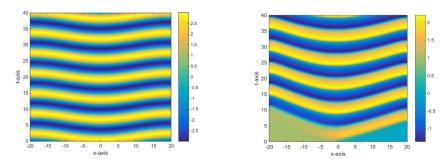


Fig. 3 Example 3, Desired periodic pattern  $u_d$  (left) and computed optimal state u (right).

Remark 5 In this and in the next examples, we fix  $t_1 = 0$ . We observed in our computational examples that the optimization with respect to  $(\kappa, t_2)$  and  $t_1 = 0$  yields sufficiently good results. Moreover, we found examples, where we got the same optimal objective value of J for very different triplets  $(\kappa, t_1, t_2)$ .

The computed optimal state for Example 3 is far from the desired one. In particular, the temporal periods are very different. The reason is that the standard quadratic tracking type functional J is not able to resolve the desired periodicity. The main point is that the  $L^2$ -norm of the difference of a time-periodic function  $t \mapsto u_d(t)$  and its phase shifted function  $t \mapsto u_d(t-s)$  can be very large, although both functions have the same time period. For instance, in  $Q = (-20, 20) \times (0, 40)$  we have

$$\iint_{Q} \left( 3 \sin(t - \cos(\frac{\pi}{20}(x+20))) - 3 \sin(t - 3 - \cos(\frac{\pi}{20}(x+20))) \right)^2 dx dt = I,$$

where  $I \approx 1.4374 \cdot 10^4$ . This brought us to considering another type of objective functionals that is discussed in the next section.

#### 7 Minimizing a cross correlation type functional

The cross correlation

As Example 3 showed, we need an objective functional that better expresses our goal of approximating periodic structures. This is the *cross correlation* between u and  $u_d$ . Moreover, in the functional, we have to observe a later part of the time interval, where u already has developed its periodicity.

Let us briefly explain the meaning of the cross correlation. Assume that  $x_d : \mathbb{R} \to \mathbb{R}$  is a periodic function with (possibly not minimal) period T and  $x : [0,T] \to \mathbb{R}$  is another function; think of a function x that is identical with  $x_d$  after a time shift.

To see, if  $x_d$  and x are time shifts of each other, we consider the extremal problem

$$\min_{s \in \mathbb{R}} \int_0^T (x(t) - x_d(t+s))^2 dt. \tag{40}$$

If x and  $x_d$  are just shifted, then the minimal value in (40) should be zero by taking the correct time shift s. The functional (40) can be simplified. To this aim, we expand the integrand,

$$\int_0^T (x(t) - x_d(t+s))^2 dt = \int_0^T x^2(t) dt - 2 \int_0^T x(t) x_d(t+s) dt + \int_0^T x_d^2(t+s) dt.$$

The first integral does not depend on s. Since  $x_d$  is a T-periodic function, also the last integral is independent of the shift s. Therefore, instead of minimizing the quadratic functional above, we can solve the following problem:

$$\max_{s \in \mathbb{R}} \frac{\int_0^T x(t) x_d(t+s) dt}{\|x\|_{L^2(0,T)} \|x_d\|_{L^2(0,T)}},\tag{41}$$

where we additionally introduced a normalization. The result is the *normalized* cross correlation between x and  $x_d$ . The largest possible value in (41) is 1; in this case, both functions are collinear.

In the application to our control problems, this induces two equivalent objective functionals. The minimization problem (40) leads to the optimization problem

$$\min_{(\kappa, t_1, t_2) \in C_{\delta}} \left( \min_{s \in \mathbb{R}} \int_{Q} (u(x, t) - u_d(x, t + s))^2 dx dt + \frac{\nu}{2} \left( \kappa^2 + t_1^2 + t_2^2 \right) \right). \tag{42}$$

The other way around is an equivalent problem that uses the cross correlation,

$$\min_{(\kappa, t_1, t_2) \in C_{\delta}} J_{corr}(\kappa, t_1, t_2) \tag{43}$$

where

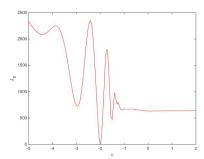
$$J_{corr}(\kappa, t_1, t_2) := 1 - \max_{s \in \mathbb{R}} \frac{\iint_Q u(x, t) u_d(x, t + s) dx dt}{\|u\|_{L^2(Q)} \|u_d\|_{L^2(Q)}} + \frac{\nu}{2} \left(\kappa^2 + t_1^2 + t_2^2\right). \tag{44}$$

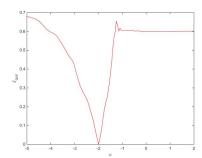
In our applications, we use the cross-correlation functional also in cases, where T is not exactly a multiple of the (minimal) period of  $u_d$ . Here, the objective functionals (43) and (42) are not completely equivalent.

For solving (43), we applied the MATLAB code pattern search that turned out to be fairly efficient in finding global minima for functions that exhibit multiple local minima. In the periodic case, we have to deal with multiple local minima indeed. Here, the cross correlation based functional  $J_{corr}$  is more useful, as the next figure shows.

Example 4 (Multiple local minima) We pre-compute the desired state by  $u_d = u_{(-2,0,2.5)}$  and consider the functions  $\kappa \mapsto J_S(\kappa,0,2.5)$  and  $\kappa \mapsto J_{corr}(\kappa,0,2.5)$  for  $\kappa$  around the (optimal) parameter  $\bar{\kappa} = -2$ .

The two functions defined in Example 4 are shown in Fig. 4. The function  $\kappa \mapsto J_S(\kappa, 0, 2.5)$  behaves more wildly around  $\kappa = -2$  than the function  $\kappa \mapsto J_{corr}(\kappa, 0, 2.5)$  that is based upon the cross correlation.





**Fig. 4** Example 4, goal functions  $\kappa \mapsto J_S(\kappa, 0, 2.5)$  (left) and  $\kappa \mapsto J_{corr}(\kappa, 0, 2.5)$  (right).

Let us re-consider the optimization problem of Example 3, but now by the cross correlation based optimization problem (43). Here, we apply the following strategy: We keep  $t_1=0$  fixed and optimize only with respect to  $(\kappa,t_2)$ . Moreover, at the beginning we fixed  $\kappa=-2$  and optimized with respect to  $\kappa$  in a second run. The computed solution was  $t_2=2.763$  with a value  $J_{corr}=0.1604, (t_1=0, \kappa=-2)$ ; as before the Tikhonov parameter was selected as  $\nu=0$ . The computed u of this first step is shown in Fig. 5. Now the agreement, in particular of the temporal period, is much better.

Next, we performed an alternating search for  $(\kappa, t_2)$  starting with the result obtained in the first step. We obtained  $t_2 = 2.7631$ ,  $\kappa = -2.4318$  and the improved objective value  $J_{corr} = 0.1229$ . This improvement is graphically hardly to distinguish from Fig. 5.

Finally, we consider another example with synthetic  $u_d$  that has a larger period than  $u_d$  of Example 3.

Example 5 We consider again  $\Omega = (-20, 20)$  and observe  $u_d$  only in the time interval [20, 40]. For  $u_d$  we select

$$u_d(x,t) = 3 \sin\left(\frac{t}{2} - \cos\left(\frac{\pi}{20}(x+20)\right)\right).$$

Again,  $t_1=0$  is fixed and the iteration is started with  $t_2=2$ ,  $\kappa=-2$ . The optimal control parameters are  $t_2=6.9419$ ,  $\kappa=-2.2837$  with computed optimal objective value  $J_{corr}=0.1209$ . The computed optimal state is shown in Fig. 6.

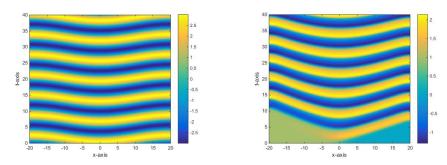


Fig. 5 Example 3, Desired pattern  $u_d$  (left) and computed pattern after minimizing  $J_{corr}$  with respect to  $t_2$  (right) for fixed  $\kappa = -2$ ,  $t_1 = 0$ .

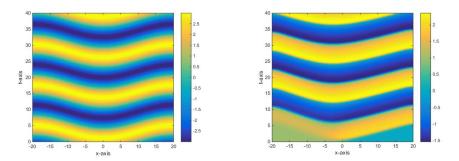


Fig. 6 Example 5, desired pattern  $u_d$  (left) and optimal pattern (right) for fixed  $t_1 = 0$ .

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